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A STOCHASTIC FRAMEWORK FOR MULTISCALE STRENGTH PREDICTION USING ADAPTIVE DISCONTINUITY LAYOUT OPTIMISATION (ADLO)

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Abstract. The prediction of strength properties of matrix-inclusion materials, which in general are random in nature due to their spatial distribution and variation of pores, particles, and matrix-inclusion interfaces, plays an important role with regard to the reliability of materials and structures. The recently developed discontinuity layout optimisation (DLO) [18] and adaptive discontinuity layout optimisation (ADLO) [4], which can be used for determination of strength properties of materials [3, 4] and structures [9], are included in a stochastic framework, using random variables. Therefore different material properties, influencing the overall strength of the matrix-inclusion material (e.g. matrix and inclusion strength, number and distribution of pores/particles) in a considered RVE are assumed to follow certain probability distributions [12]. A sensitivity study for the identification of material parameters showing the largest influence on the strength of the considered matrix-inclusion materials is performed. The obtained results provide first insight into the nature of the reliability of strength properties of matrix-inclusion materials, paving the way to a better understanding and finally improvement of the effective strength properties of matrix-inclusion materials.

1 INTRODUCTION

As engineering materials, such as composites and heterogeneous high strength - low weight materials, are continuously improving in engineering applications (e.g. aerospace, mechanical-engineering, civil-engineering, etc.), allowing their application in high-performance structures (e.g. airplanes, lightweight cars, high-rise buildings), the proper identification and understanding of the underlying effective strength properties are of crucial importance. Since the microstructure of these matrix-inclusion materials (e.g.

ultra-high performance concrete, carbon fibre-reinforced materials, etc.) is in general random in nature with varying spatial distribution, size, and shape of pores, particles, and matrix-inclusion interfaces, a statistical framework is necessary in the model-based analysis, characterization and finally prediction of material properties, see for instance [13, 1, 8, 7, 10, 11, 12, 14, 16]. Hereby, the description of the random microstructure defines the quality of the employed model and, hence, strongly influences the obtained results. In addition to the volume fractions of reinforcing inclusions (e.g. particles and fibres), their shape and more importantly their spatial arrangement are thought to strongly affect the strength properties of composite materials [17].
The underlying methodology of the finite element method (FEM), employing nodes and finite elements for the spatial description of the material system under consideration, offers the possibility to represent the microstructure of composite materials in an appropriate manner. Accordingly, the FEM was successfully applied e.g. in [2] to predict the stress distribution inside the inclusion of RVEs containing a number of randomly oriented elliptical inclusions, and in [5] for the representation of microstructures with varying particle volume fractions, particle locations, and constituent material properties following a stochastic description in order to determine the fracture behaviour of functionally-graded materials. In [19], the same approach was chosen for determination of the damage behaviour of concrete using a model with random aggregate structure at the mesoscopic level. Disadvantages of the FEM such as the dependency of the results on the discretization and unsatisfactory modelling of the interface behaviour between inclusions and the matrix material were highlighted in [19]. In contrast to the numerical approach of the FEM, a continuum micromechanics-based approach, employing the concept of limit stress states, is proposed in [15], taking into account a random two-phase heterogeneous microstructure, giving access to the effective yield function and, hence, to strength properties of composite materials. However, neither the spatial arrangement of the inclusions within the RVE, nor the variation of shape of the inclusions are considered in this approach.
As a remedy, the recently developed discontinuity layout optimisation (DLO) [18] and adaptive discontinuity layout optimisation (ADLO) [3] provides a methodology, considering the detailed microstructure of random heterogeneous materials. First obtained results for the strength of matrix-inclusion materials using unit cells as well as representative volume elements (RVE) for porous materials showed good agreement with analytical results [4]. As a probabilistic extension of the ADLO, a framework using stochastic limit analysis for matrix-inclusion materials with varying material properties and morphologies (e.g. matrix and inclusion strength, number, shape and distribution of pores/inclusions) following certain probability distributions is proposed in this paper. The so-obtained results provide first insight into the nature of strength properties of matrix-inclusion materials with different volume fractions of circular and elliptical inclusion and varying strength properties of the matrix, particles, and matrix-inclusion interfaces, paving the way to a better understanding and finally improvement of effective strength properties of matrix-

inclusion materials.

2 Methodology

In this work, the recently developed ADLO [4, 3], as a limit analysis methodology, is used to predict the strength properties of matrix-inclusion materials. The heterogeneous morphology of the material is discretized with a random set of n nodes, whereas the discontinuities are generated as lines between these nodes by the delaunay triangulation [6]. Hereby, every discontinuity can be assigned to a certain material model, therein, the Mohr-Coulomb material model with the cohesion c and the angle of friction ϕ is considered, taking into consideration different material properties for the matrix, inclusions, and interfaces. Every discontinuity may be a potential failure discontinuity and, thus, contribute to the failure mode. By employing linear programming, the set of failed discontinuities is calculated which yields the minimized internal energy of the material system, resulting in an upper-bound (UB) formulation with the following linear programming (LP) problem (for details, see [18, 3, 4]):

$$\min \lambda \mathbf{f}_L^T \mathbf{d} = -\mathbf{f}_D^T \mathbf{d} + \mathbf{g}^T \mathbf{p},$$

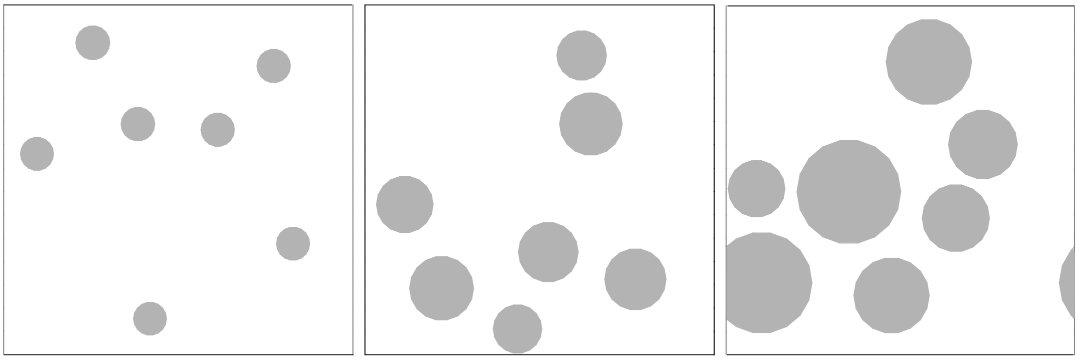
subject to

$$\begin{aligned} \mathbf{Bd} &= \mathbf{0}, \\ \mathbf{f}_L^T \mathbf{d} &= 1, \\ \mathbf{Np} - \mathbf{d} &= \mathbf{0}, \\ \mathbf{p} &\geq \mathbf{0}, \end{aligned} \tag{1}$$

where $\mathbf{f}_L$ [N] and $\mathbf{f}_D$ [N] are $(2m)$ vectors containing the shear and normal component for live and dead load, respectively, and λ is the failure load-factor, $\mathbf{g}$ [N] is the $(2m)$ vector containing the product of length ℓ [m] and cohesive shear strength c [N/m] of the discontinuities, $\mathbf{B}$ [-] is a $(2n$ x $2m)$ compatibility matrix, and $\mathbf{N}$ [-] is a $(2m$ x $2m)$ plastic-flow matrix. In Equation (1), $\mathbf{d}$ and $\mathbf{p}$ represent the unknowns of the LP problem, where $\mathbf{d}$ [m] is a $(2m)$ vector of discontinuity displacements, and $\mathbf{p}$ [m] is a $(2m)$ vector of plastic multipliers.

Given the optimization problem in Equation (1), the statistical framework for matrix-inclusion materials is established, considering three aspects of material morphology:

- First, the mean strength $\bar{f}_t$ of an RVE with seven circular, randomly-distributed inclusions subjected to uniaxial tension is predicted. Hereby, the inclusion strength $\bar{f}_t^{Inc}$ is chosen 100 times the matrix strength f_t^M and the interfaces strength $\bar{f}_t^{Int}$ is set equal to the matrix strength f_t^M. The volume fraction of the inclusions, f_a, is varied from 0.05 to 0.3. Moreover, for each volume fraction different inclusion radii are considered within an RVE, characterized by the mean value and the standard



(a) (b) (c)

Figure 1: RVEs with seven circular inclusions: (a) $f_a = 0.05$, $s_r = 0.01$, (b) $f_a = 0.15$, $s_r = 0.1$, and (c) $f_a = 0.3$, $s_r = 0.2$

deviation s_r of the radii, with s_r varying from 0.01 to 0.3, taking the grading of the inclusions into account. Figure 1 shows three different layouts for the RVE.

- In a second study, the influence of interface strength $\bar{f}_t^{Int}$ on the effective strength of an RVE with seven circular, randomly-distributed inclusions subjected to uniaxial tension is investigated. For this purpose, $\bar{f}_t^{Int}$ is varied from 10 to 100 % of the matrix strength, with $f_a = 0.05, 0.15, 0.3$ and $s_r = 0.01$.

- Finally, an RVE with seven randomly-distributed and randomly-oriented elliptical inclusions subjected to uniaxial tension is considered. The material properties are the same as in the first study. The volume fraction of the inclusions f_a is varied within 0.05, 0.15, 0.3 and the ellipse eccentricity E from 1 to 7. Figure 2 shows three different layouts for randomly-generated RVEs.

For all studies reported in this paper, 500 different randomly-generated RVEs were considered for each set of parameters.

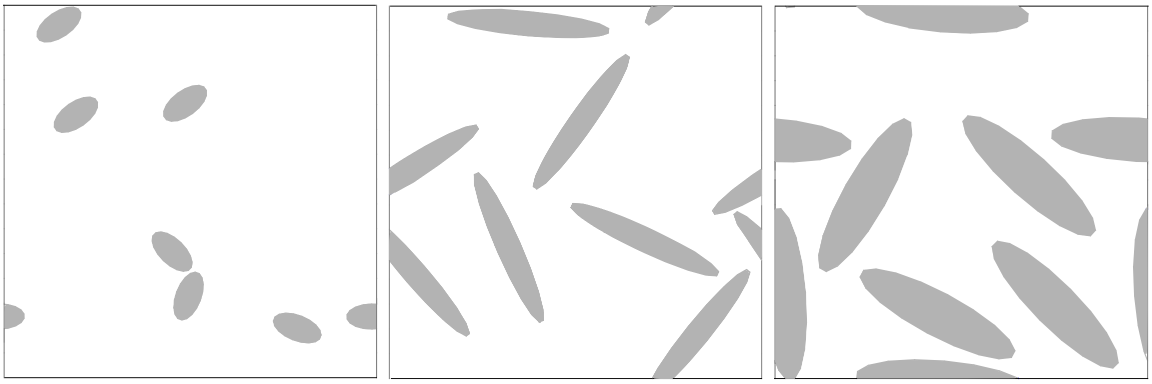

(a) (b) (c)

Figure 2: RVEs with seven elliptical inclusions: (a) $f_a = 0.05$, $E = 2$, (b) $f_a = 0.15$, $E = 7$, and (c) $f_a = 0.3$, $E = 4$

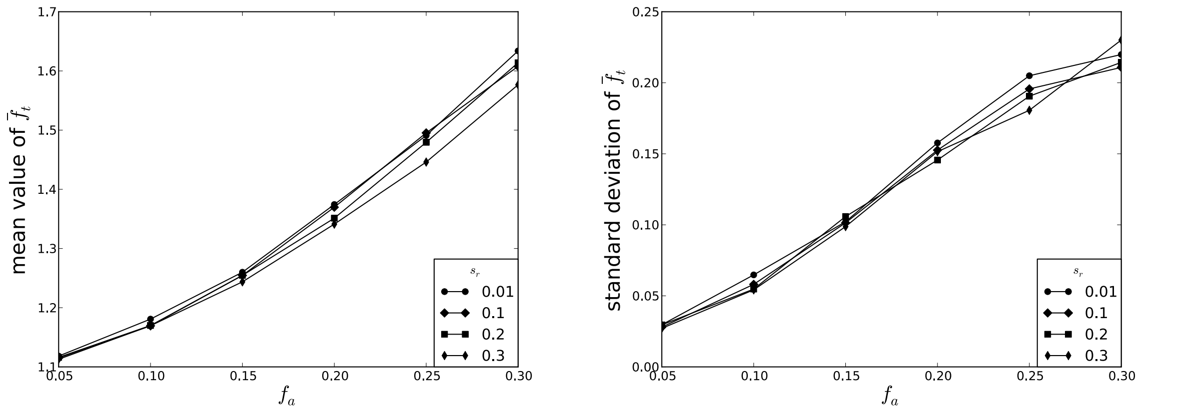
3 Results and discussion

In this section, the proposed stochastic framework for strength homogenisation is applied to the three different aspects of matrix inclusion materials: First, the effective strength properties of materials with circular particles of varying size are investigated. Subsequently, the effect of decreasing interface properties on the effective strength is shown. Finally, the effective material strength properties of RVEs containing elliptical particles are discussed.

Circular particles and constant interface strength

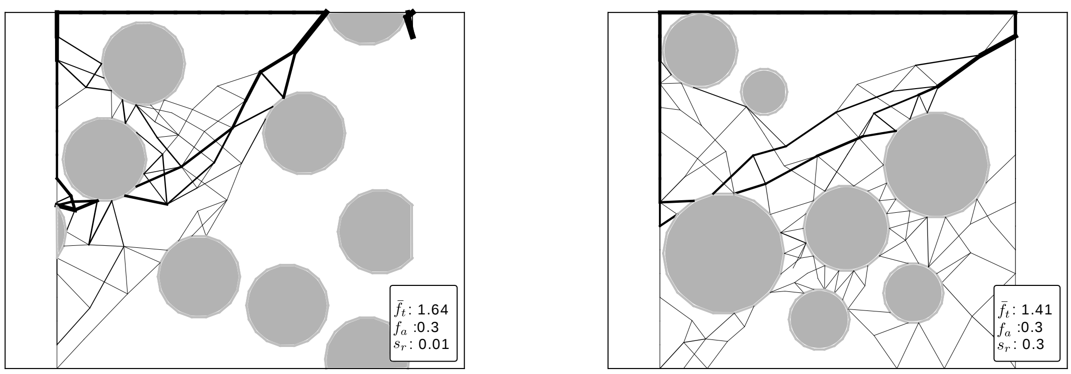
Figure 3(a) shows the mean value of the effective tensile strength $\bar{f}_t$ as a function of f_a for different values of s_r. As expected, the mean value of $\bar{f}_t$ of the investigated RVEs increases with increasing volume fraction of the particles f_a. Also the influence of s_r on the mean value of $\bar{f}_t$ increases with increasing f_a, giving lower values for the effective tensile strength for larger variation of the particle size. This slight decrease can be explained by the increasing distance between inclusions with increasing particle variation, enabling the failure mechanism to develop between inclusions within the weaker matrix material (see Figure 4).

Also the standard deviation of $\bar{f}_t$ increases with increasing f_a as illustrated in Figure 3(b). This is explained by the random spatial arrangement of the particles within the RVEs with high f_a generating morphologies enabling both blocking of the failure mode by particles (Figure 5(a)) and the development of the failure mechanism between the particles (Figure 5(b)) within the weaker matrix material. In case of low volume fractions of particles, on the other hand, the failure mode most likely develops within the matrix (see Figure 5(c)), explaining the low value of the standard deviation of $\bar{f}_t$. A trend for the influence of s_r on the standard deviation of $\bar{f}_t$, on the other hand, could not be observed.



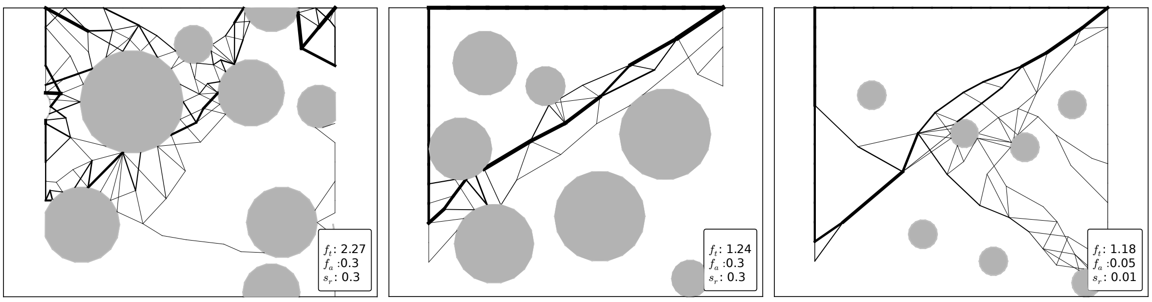
(a) (b)

Figure 3: Circular particles: (a) Mean value and (b) standard deviation of $\bar{f}_t$ as a function of s_r and f_a ($f_t^M = 1$, $\bar{f}_t^{Int} = f_t^M$, $\bar{f}_t^{Inc} = 100$)



(a) (b)

Figure 4: Circular particles: Failure modes of RVEs with $f_a = 0.3$ and (a) $s_r = 0.01$ and (b) $s_r = 0.3$



(a) (b) (c)

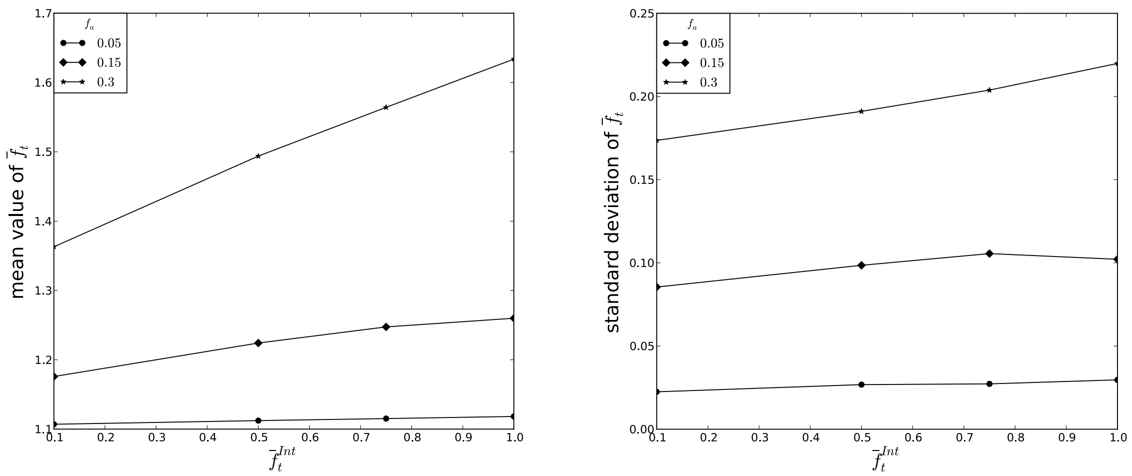
Figure 5: Circular particles: Failure modes of RVEs with (a) $f_a = 0.3$, $s_r = 0.3$, (b) $f_a = 0.3$, $s_r = 0.3$, and (c) $f_a = 0.05$, $s_r = 0.1$

Variation of interface properties

In Figure 6(a), the mean value of $\bar{f}_t$ with respect to $\bar{f}_t^{Int}$ for different f_a is given, indicating almost no effect of $\bar{f}_t^{Int}$ on $\bar{f}_t$ for low volume fractions of particles. This is explained by the development of the failure mechanism within the matrix phase passing between the particles, resulting in low values of $\bar{f}_t$. For high volume fractions of the particles, on the other hand, the particle phase and, hence, the interface properties become dominant, resulting in higher values for $\bar{f}_t$ (see Figure 6(a)). The marginal effect of $\bar{f}_t^{Int}$ on the standard deviation of $\bar{f}_t$ is explained by $\bar{f}_t^{Int}$ affecting only the failure load via the vector $\mathbf{g}$ in the objective function (Equation (1)) and not the failure mechanism, which is specified by the constraints in Equation (1).

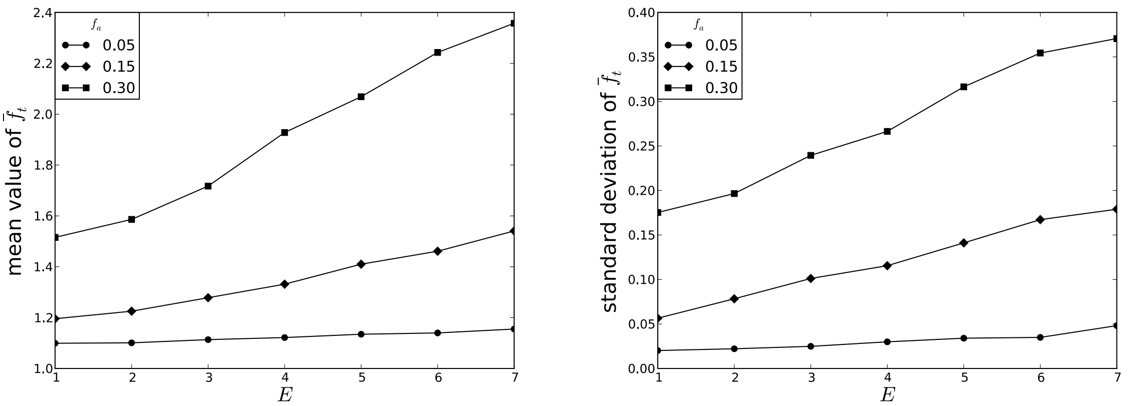
Elliptical particles

Figure 7(a) shows the mean value of $\bar{f}_t$ as a function of E for different values of f_a. As expected, the mean value of $\bar{f}_t$ of the investigated RVEs increases with increasing E. This increase is more pronounced for higher volume fractions of particles, leading to an increase of the length of the failure mechanism (see Figure 8) with long elliptical inclusions blocking the development of the failure mechanism. With increasing E, the values of the standard deviation of $\bar{f}_t$ increases (see Figure 7(b)). This observation is explained by different orientations of elliptical inclusions either blocking (high-strength configuration, horizontal alignment in Figure 9(a)) or enabling the failure mechanism to develop between the inclusions within the weaker matrix material (low-strength configuration, alignment with the expected failure angle of the matrix $\approx 45°$ in Figure 9(b)).



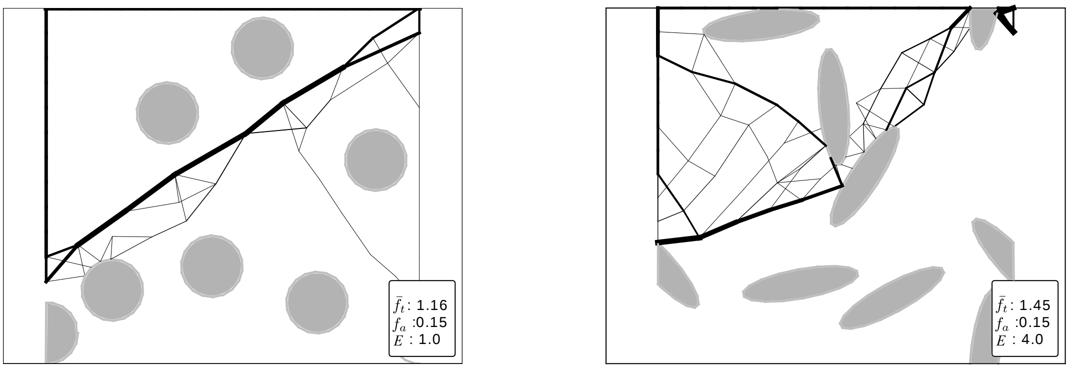
(a) (b)

Figure 6: Variation of interfaces properties: (a) Mean value and (b) standard deviation of $\bar{f}_t$ as a function of f_a and $\bar{f}_t^{Int}$ ($f_t^M = 1$, $\bar{f}_t^{Inc} = 100$)



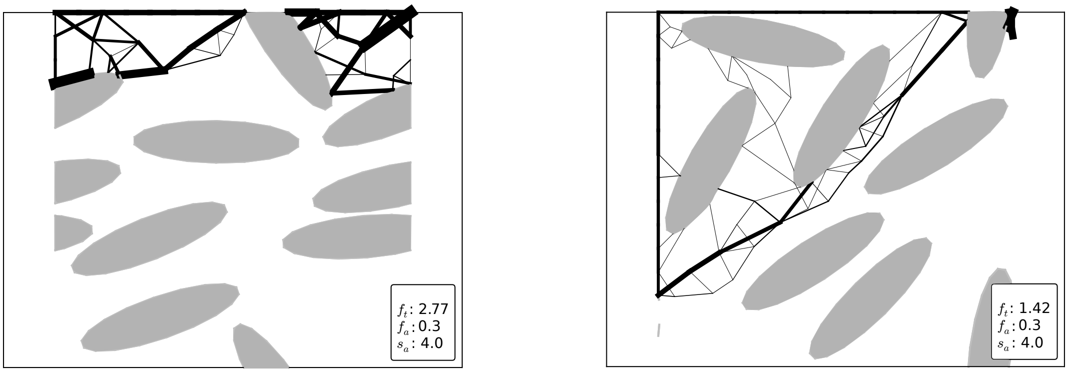
(a) (b)

Figure 7: Elliptical particles: (a) Mean value and (b) standard deviation of $\bar{f}_t$ as a function of E for different f_a ($f_t^M = 1$, $\bar{f}_t^{Int} = \bar{f}_t^M$, $\bar{f}_t^{Inc} = 100$)



(a) (b)

Figure 8: Elliptical particles: Failure mechanisms of RVEs with $f_a = 0.15$ and (a) $E = 1$ and (b) $E = 4$



(a) (b)

Figure 9: Elliptical particles: Failure mechanisms of RVEs with $f_a = 0.3$ and $E = 4$ with (a) high-strength and (b) low-strength configuration

4 Conclusion

In this work, a statistical framework using stochastic limit analysis was proposed for the prediction of effective strength properties of matrix-inclusion materials with randomly distributed/oriented circular and elliptical particles, employing adaptive discontinuity layout optimisation (ADLO) [3]. Based on the results of the performed studies, the following conclusions can be drawn:

- The mean value of the effective strength of the considered heterogeneous matrix-inclusion material mainly depends on the length of the failure mode. An increase in length may be accomplished by the increase of particle content and/or the use of elliptical particles with high eccentricity ratio.
- In case of particles blocking the development of the failure mechanism, the interface properties become increasingly important, affecting the effective strength of the composite material.
- The standard deviation of the effective strength follows the trend of the mean value, giving increasing standard deviation for increasing particle content. This corresponds well to the aforementioned influence of the length of the failure mechanism, ranging from a straight line in case of failure in the matrix phase to a maximum length depending on the particle content.
- Finally, higher variation in particle size results in an increase of the interparticle face-to-face distance (as illustrated in Figure 10), providing more space for the failure mechanism to develop within the matrix material. This yields a lower mean value for the effective strength even though the volume fraction of particles remains constant.

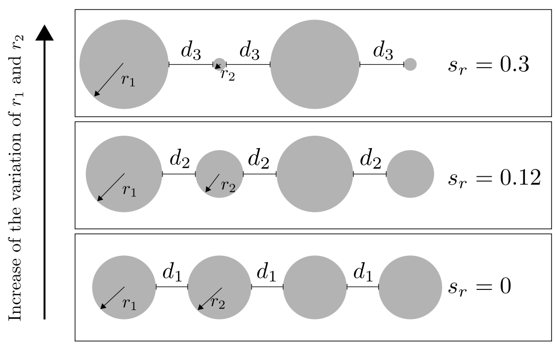


Figure 10: Interparticle distance for varying particle radius with constant volume fraction: $d_1 = 0.5$, $d_2 = 0.52$, and $d_3 = 0.7$

Having developed a statistical framework providing first insight into the nature and the reliability of strength properties of matrix-inclusion materials, future work will include the consideration of materials with randomly distributed pores with varying shape and orientation. Finally, the ADLO shall be extended towards three-dimensional applications.

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